

10563975

NEWS IPC8 For general information regarding STN implementation of IPC 8
NEWS X25 X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 09:50:09 ON 21 FEB 2007

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 09:50:16 ON 21 FEB 2007

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DICTIONARY FILE UPDATES: 19 FEB 2007 HIGHEST RN 921921-74-6

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<http://www.cas.org/ONLINE/UG/regprops.html>

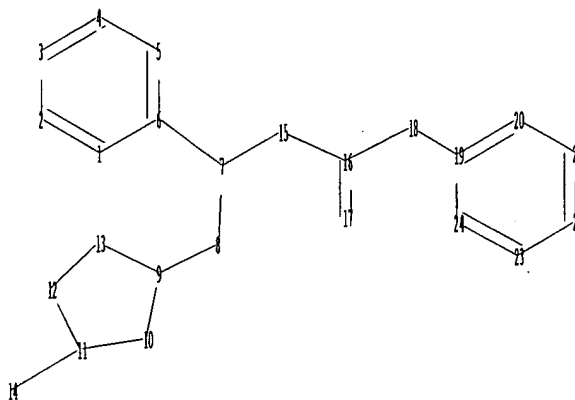
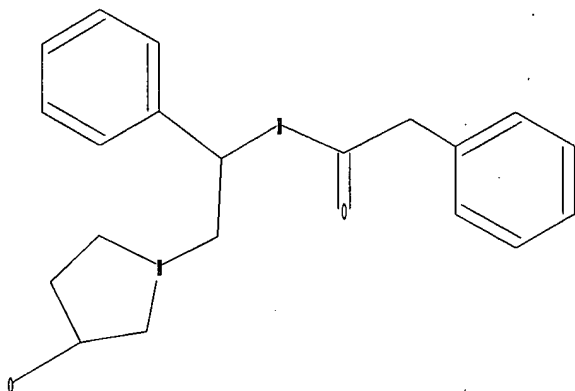
=>

Uploading C:\Program Files\Stnexp\Queries\10563975.str

Karen Cheng

10563975

broapest search



chain nodes :

7 8 14 15 16 17 18

ring nodes :

1 2 3 4 5 6 9 10 11 12 13 19 20 21 22 23 24

chain bonds :

6-7 7-8 7-15 8-9 11-14 15-16 16-17 16-18 18-19

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-13 10-11 11-12 12-13 19-20 19-24 20-21
21-22 22-23 23-24

exact/norm bonds :

7-15 8-9 9-10 9-13 11-14 15-16 16-17

exact bonds :

6-7 7-8 10-11 11-12 12-13 16-18 18-19

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 19-20 19-24 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 9 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:Atom

11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom

L1 STRUCTURE UPLOADED

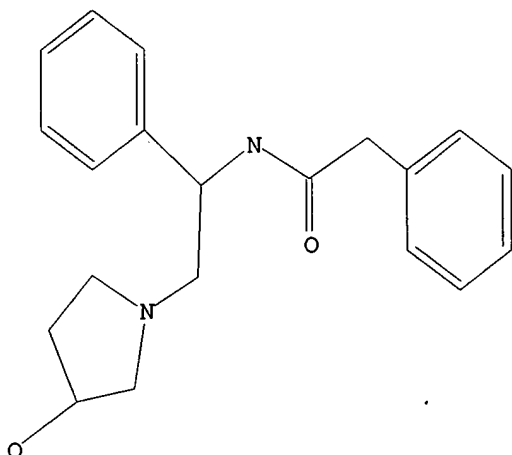
=> d

L1 HAS NO ANSWERS

L1 STR

Karen Cheng

10563975



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 09:50:39 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1304 TO ITERATE

100.0% PROCESSED 1304 ITERATIONS

359 ANSWERS

SEARCH TIME: 00.00.01

L2 359 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

172.10

172.31

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<http://www.cas.org/infopolicy.html>

=> s 12

L3 83 L2

=> fil stng

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.47	172.78

FULL ESTIMATED COST

FILE 'STNGUIDE' ENTERED AT 09:50:53 ON 21 FEB 2007
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FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Feb 16, 2007 (20070216/UP).

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.18	172.96

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 09:52:44 ON 21 FEB 2007
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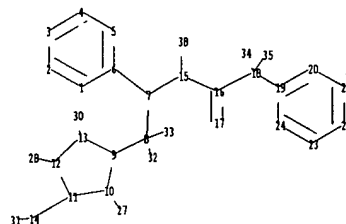
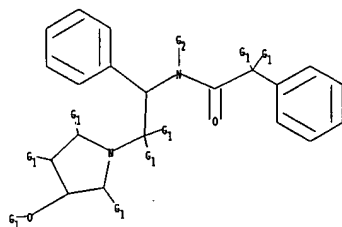
<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10563975a.str...

Karen Cheng

limit H substituents to H; Me



chain nodes :

7 8 14 15 16 17 18 27 28 30 31 32 33 34 35 38

ring nodes :

1 2 3 4 5 6 9 10 11 12 13 19 20 21 22 23 24

chain bonds :

6-7 7-8 7-15 8-9 8-32 8-33 10-27 11-14 12-28 13-30 14-31 15-16 15-38
16-17 16-18 18-19 18-34 18-35

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-13 10-11 11-12 12-13 19-20 19-24 20-21
21-22 22-23 23-24

exact/norm bonds :

7-15 8-9 8-32 8-33 9-10 9-13 10-27 11-14 12-28 13-30 14-31 15-16 15-38
16-17 18-34 18-35

exact bonds :

6-7 7-8 10-11 11-12 12-13 16-18 18-19

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 19-20 19-24 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 9 :

G1:H,CH3

G2:H,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 27:CLASS 28:CLASS 30:CLASS
31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 38:CLASS

L4

STRUCTURE UPLOADED

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=> d his

(FILE 'HOME' ENTERED AT 09:50:09 ON 21 FEB 2007)

FILE 'REGISTRY' ENTERED AT 09:50:16 ON 21 FEB 2007

L1 STRUCTURE UPLOADED
L2 359 S L1 FULL

FILE 'CAPLUS' ENTERED AT 09:50:48 ON 21 FEB 2007

L3 83 S L2

FILE 'STNGUIDE' ENTERED AT 09:50:53 ON 21 FEB 2007

FILE 'REGISTRY' ENTERED AT 09:52:44 ON 21 FEB 2007
L4 STRUCTURE UPLOADED

=> s 14 full sub=12

FULL SUBSET SEARCH INITIATED 09:53:26 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 359 TO ITERATE

100.0% PROCESSED 359 ITERATIONS 253 ANSWERS
SEARCH TIME: 00.00.01

L5 253 SEA SUB=L2 SSS FUL L4

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	41.10	214.06

FILE 'CAPLUS' ENTERED AT 09:53:35 ON 21 FEB 2007
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=> s 15

L6 78 L5

=> fil stng

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.47	214.53

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	214.95

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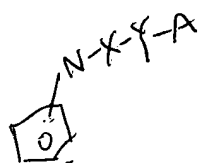
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=>

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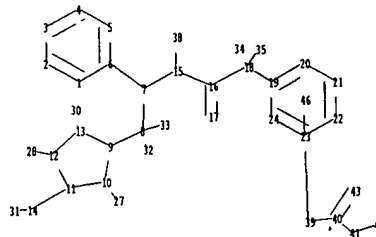
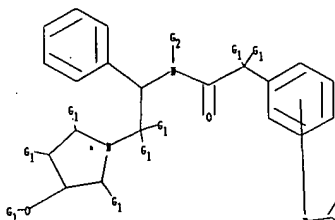


add -N substituent off benzene ring.

X = CO. or CS

Y = O, NH, CH₂

A = Cy



Cy = ring systems.

chain nodes :

7 8 14 15 16 17 18 27 28 30 31 32 33 34 35 38 39 40 41 42 43

ring nodes :

1 2 3 4 5 6 9 10 11 12 13 19 20 21 22 23 24

chain bonds :

6-7 7-8 7-15 8-9 8-32 8-33 10-27 11-14 12-28 13-30 14-31 15-16 15-38
16-17 16-18 18-19 18-34 18-35 39-40 40-41 40-43 41-42

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-13 10-11 11-12 12-13 19-20 19-24 20-21
21-22 22-23 23-24

exact/norm bonds :

7-15 8-9 8-32 8-33 9-10 9-13 10-27 11-14 12-28 13-30 14-31 15-16 15-38
16-17 18-34 18-35 39-40 40-41 40-43 41-42

exact bonds :

6-7 7-8 10-11 11-12 12-13 16-18 18-19

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 19-20 19-24 20-21 21-22 22-23 23-24

isolated ring systems :

containing 1 : 9 :

G1:H,CH3

G2:H,Ak

G3:C,O,N

G4:O,S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 27:CLASS 28:CLASS 30:CLASS
31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 38:CLASS 39:CLASS 40:CLASS
41:CLASS 42:Atom 43:CLASS 46:Atom

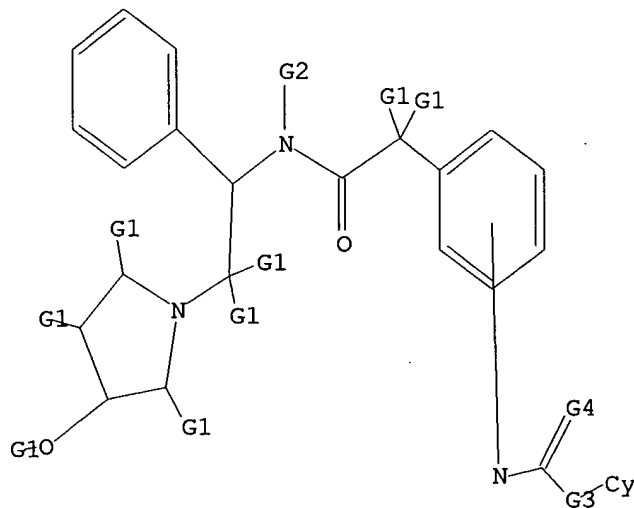
10563975

L7 STRUCTURE UPLOADED

=> d

L7 HAS NO ANSWERS

L7 STR



G1 H, Me

G2 H, Ak

G3 C, O, N

G4 O, S

Structure attributes must be viewed using STN Express query preparation.

=> s 17 full

FULL SEARCH INITIATED 09:58:03 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 793 TO ITERATE

100.0% PROCESSED 793 ITERATIONS

12 ANSWERS

SEARCH TIME: 00.00.01

L8 12 SEA SSS FUL L7

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

172.10

387.05

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=> s l8

L9 1 L8

=> d ibib abs hitstr tot

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=> fil reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
5.74	570.69

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.78	-1.56

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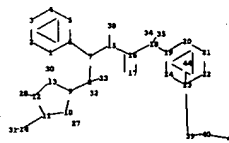
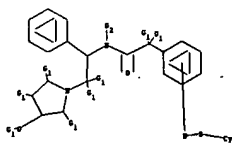
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=>

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```
chain nodes :
7 8 14 15 16 17 18 27 28 30 31 32 33 34 35 38 39 40 41
ring nodes :
1 2 3 4 5 6 9 10 11 12 13 19 20 21 22 23 24
chain bonds :
6-7 7-8 7-15 8-9 8-32 8-33 10-27 11-14 12-28 13-30 14-31 15-16 15-38
16-17 16-18 18-19 18-34 18-35 39-40 40-41
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-13 10-11 11-12 12-13 19-20 19-24 20-21
21-22 22-23 23-24
exact/norm bonds :
7-15 8-9 8-32 8-33 9-10 9-13 10-27 11-14 12-28 13-30 14-31 15-16 15-38
16-17 18-34 18-35 39-40 40-41
exact bonds :
6-7 7-8 10-11 11-12 12-13 16-18 18-19
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 19-20 19-24 20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 9 :
```

G1:H,CH3

G2:H,Ak

G3:C,O,N

G4:O,S

Match level :

```
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 27:CLASS 28:CLASS 30:CLASS
31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 38:CLASS 39:CLASS 40:CLASS
41:Atom 44:Atom
```

L13 STRUCTURE UPLOADED

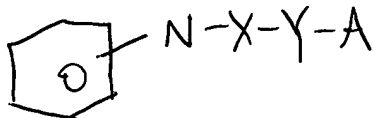
=> d

L13 HAS NO ANSWERS

L13 STR

Karen Cheng

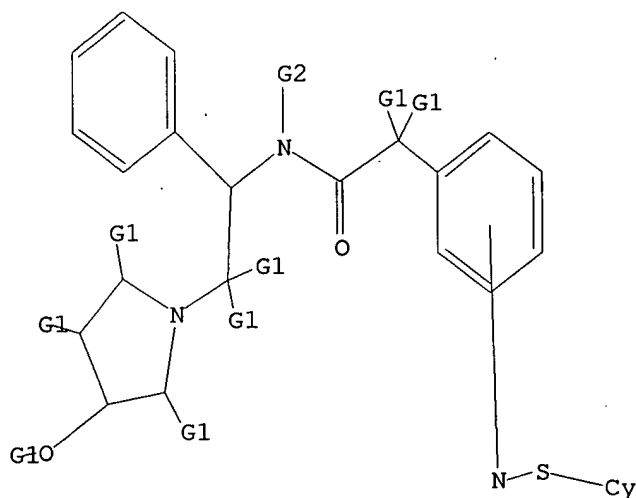
10563975



X = SO₂

Y = single bond

A = Cy = ring systems



G1 H, Me

G2 H, Ak

G3 C, O, N

G4 O, S

Structure attributes must be viewed using STN Express query preparation.

=> d his

(FILE 'HOME' ENTERED AT 09:50:09 ON 21 FEB 2007)

FILE 'REGISTRY' ENTERED AT 09:50:16 ON 21 FEB 2007

L1 STRUCTURE UPLOADED

L2 359 S L1 FULL

FILE 'CAPLUS' ENTERED AT 09:50:48 ON 21 FEB 2007

L3 83 S L2

FILE 'STNGUIDE' ENTERED AT 09:50:53 ON 21 FEB 2007

FILE 'REGISTRY' ENTERED AT 09:52:44 ON 21 FEB 2007

L4 STRUCTURE UPLOADED

L5 253 S L4 FULL SUB=L2

FILE 'CAPLUS' ENTERED AT 09:53:35 ON 21 FEB 2007

L6 78 S L5

FILE 'STNGUIDE' ENTERED AT 09:53:41 ON 21 FEB 2007

FILE 'REGISTRY' ENTERED AT 09:57:36 ON 21 FEB 2007

L7 STRUCTURE UPLOADED

L8 12 S L7 FULL

Karen Cheng

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FILE 'CAPLUS' ENTERED AT 09:58:09 ON 21 FEB 2007
L9 1 S L8

FILE 'STNGUIDE' ENTERED AT 09:58:38 ON 21 FEB 2007

FILE 'REGISTRY' ENTERED AT 09:59:29 ON 21 FEB 2007
L10 STRUCTURE UPLOADED
L11 4 S L10 FULL

FILE 'CAPLUS' ENTERED AT 10:00:04 ON 21 FEB 2007
L12 1 S L11

FILE 'REGISTRY' ENTERED AT 10:00:20 ON 21 FEB 2007
L13 STRUCTURE UPLOADED

=> s l13 full sub=15

FULL SUBSET SEARCH INITIATED 10:01:38 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 76 TO ITERATE

100.0% PROCESSED 76 ITERATIONS 25 ANSWERS
SEARCH TIME: 00.00.01

L14 25 SEA SUB=L5 SSS FUL L13

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
41.55	612.24

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-1.56

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=> s l14

L15 1 L14

=> d ibib abs hitstr tot